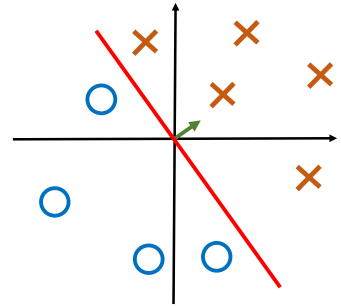
Support Vector Machines

CISC 5800
Professor Daniel Leeds

Separating boundary, defined by **w**



- Separating **hyperplane** splits **class 0** and **class 1**
- Plane is defined by line **w** perpendicular to plan
- Is data point **x** in class 0 or class 1? $\mathbf{w}^T\mathbf{x}+b > 0$ class **1**
  $\mathbf{w}^T\mathbf{x}+b < 0$ class **0**

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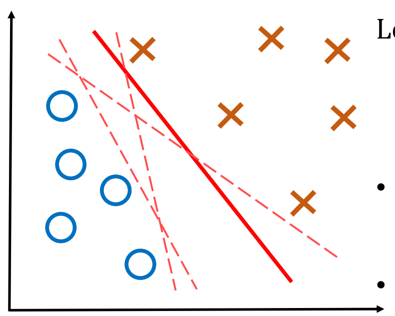
But, where do we place the boundary?



Logistic regression:

$$LL(y|x;w): \sum_i (y^i - 1)\boldsymbol{w}^T\boldsymbol{x}^i - \log\left(1 + e^{-\boldsymbol{w}^T\boldsymbol{x}^i}\right)$$

- Each data point $\boldsymbol{x}^i$ considered for boundary $\boldsymbol{w}$
- Outlier data pulls boundary towards it

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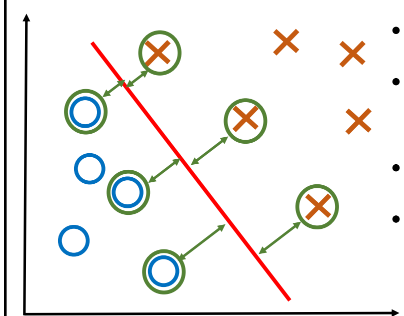
Max margin classifiers



- Focus on boundary points
- Find largest margin between boundary points on both sides
- Works well in practice
- We can call the boundary points **"support vectors"**

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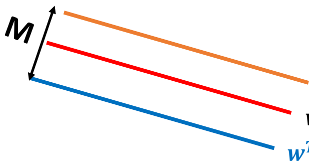
Maximum margin definitions



Classify as +1
if $w^T x + b \geq 1$

Classify as -1
if $w^T x + b \leq -1$

Undefined
if $-1 \leq w^T x + b \leq 1$

- M is the margin width
- x^+ is a +1 point closest to boundary, x^- is a -1 point closest to boundary
- $x^+ = \lambda w + x^-$
- $|x^+ - x^-| = M$

$$M = \frac{2}{\sqrt{w^T w}}$$

maximize M **minimize $w^T w$**

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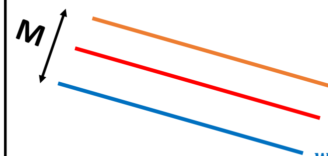
λ derivation

Optional extra math



- $w^T x^- + b = -1$
- $w^T x^+ + b = +1$
- $x^+ = \lambda w + x^-$

- $w^T x^+ + b = +1$
- $w^T(\lambda w + x^-) + b = +1$
- $\lambda w^T w + w^T x^- + b = +1$
- $\lambda w^T w - 1 - b + b = +1$
- $\lambda = \frac{2}{w^T w}$

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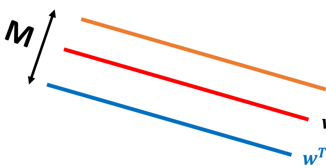
M derivation

Optional extra math



- $w^T x^- + b = -1$
- $w^T x^+ + b = +1$
- $x^+ = \lambda w + x^-$
- $|x^+ - x^-| = M$

- $M = |\lambda w + x^- - x^-| = |\lambda w| = \lambda |w|$
- $M = \lambda \sqrt{w^T w}$
- $M = \frac{2}{w^T w} \sqrt{w^T w} = \frac{2}{\sqrt{w^T w}}$

maximize M minimize $w^T w$

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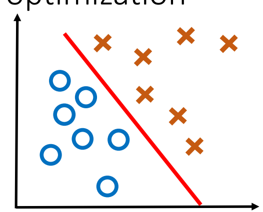
Support vector machine (SVM) optimization

$\max_w M = \frac{2}{\sqrt{w^T w}}$

$\min_w w^T w$
subject to
$w^T x + b \geq 1$ for **x** in class 1
$w^T x + b \leq -1$ for **x** in class -1



Optimization with constraints: $\frac{\partial}{\partial w_j} f(w_j) = 0$ with Lagrange multipliers.

- Gradient descent
- Matrix calculus

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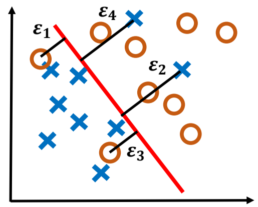
Support vector machine (SVM) optimization
with slack variables

What if data not linearly separable?



$\text{argmin}_{w,b}\ \boldsymbol{w}^T\boldsymbol{w} + C\sum_i \varepsilon^i$

subject to

$\boldsymbol{w}^T\boldsymbol{x} + b \geq 1 - \varepsilon^i$ **for x in class 1**

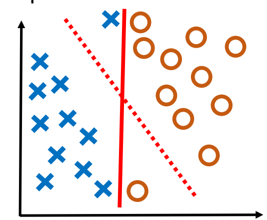
$\boldsymbol{w}^T\boldsymbol{x} + b \leq -1 + \varepsilon^i$ **for x in class -1**

$\varepsilon_i \geq 0 \quad \forall i$

Each error ε_i is penalized based on distance from separator

Support vector machine (SVM) optimization
with slack variables

Example: Linearly separable but with narrow margins



$\text{argmin}_{w,b}\ \boldsymbol{w}^T\boldsymbol{w} + C\sum_i \varepsilon^i$

subject to

$\boldsymbol{w}^T\boldsymbol{x} + b \geq 1 - \varepsilon^i$ **for x in class 1**

$\boldsymbol{w}^T\boldsymbol{x} + b \leq -1 + \varepsilon^i$ **for x in class -1**

$\varepsilon_i \geq 0 \quad \forall i$

Hyper-parameters for learning

$\text{argmin}_{w,b}\ \boldsymbol{w}^T\boldsymbol{w} + C\sum_i \varepsilon_i$

Optimization constraints: ***C*** influences tolerance for label errors versus narrow margins

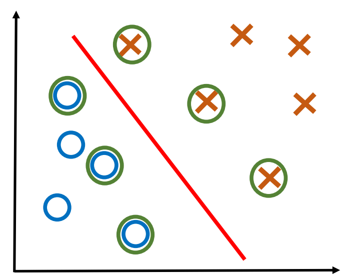
$$w_j \leftarrow w_j + \varepsilon\left[x_j^i\left(y^i - g(w^T\boldsymbol{x}^i)\right) - \frac{w_j}{\lambda N}\right]$$

Gradient ascent:

- ***ε*** influences effect of individual data points in learning
- ***T*** number of training examples, ***L*** number of loops through data – balance learning and over-fitting

Regularization: ***λ*** influences the strength of your prior belief

Alternate SVM formulation



$$\boldsymbol{w} = \sum_i \alpha^i \boldsymbol{x}^i y^i$$

Support vectors $\boldsymbol{x_i}$ have $\alpha_i > 0$

y_i are the data labels +1 or -1

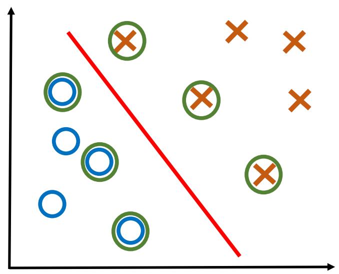
To classify sample $\mathbf{x}^k$, compute:

$$\boldsymbol{w}^T\boldsymbol{x}^k + b = \sum_i \alpha^i y^i \boldsymbol{x}^i \boldsymbol{x}^k + b$$

$\boldsymbol{\alpha^i \geq 0\ \forall i}$ $\quad \boldsymbol{\sum_i \alpha^i\ y^i = 0}$

Example

$$w = \sum_i \alpha^i x^i y^i$$



$x^1 = \begin{bmatrix}-1\\1\end{bmatrix}, y^1 = +1, \alpha^1 = 0.5$

$x^2 = \begin{bmatrix}0\\0\end{bmatrix}, y^2 = +1, \alpha^2 = 0.7$

$x^3 = \begin{bmatrix}-1\\-1\end{bmatrix}, y^3 = -1, \alpha^3 = 1$

$x^4 = \begin{bmatrix}-0.5\\-3\end{bmatrix}, y^4 = -1, \alpha^4 = 0.2$

$w =$

$0.5 \times \begin{bmatrix}-1\\1\end{bmatrix} + 0.7 \times \begin{bmatrix}0\\0\end{bmatrix} - 1 \times \begin{bmatrix}-1\\-1\end{bmatrix} - 0.2 \times \begin{bmatrix}-0.5\\-3\end{bmatrix}$

$= \begin{bmatrix}-0.5+1+0.1\\0.5+1+0.6\end{bmatrix} = \begin{bmatrix}0.6\\2.1\end{bmatrix}$

$\alpha^i \geq 0 \;\forall i$ $\quad \sum_i \alpha^i y^i = 0$

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Hyper-parameters to learn

Each data point x^i has N features (presuming classify with $w^T x^i + b$)

Separator: w and b

- N elements of **w**, 1 value for b: $N+1$ parameters **OR**
- t support vectors -> t non-zero α^i, 1 value for b: $t+1$ parameters

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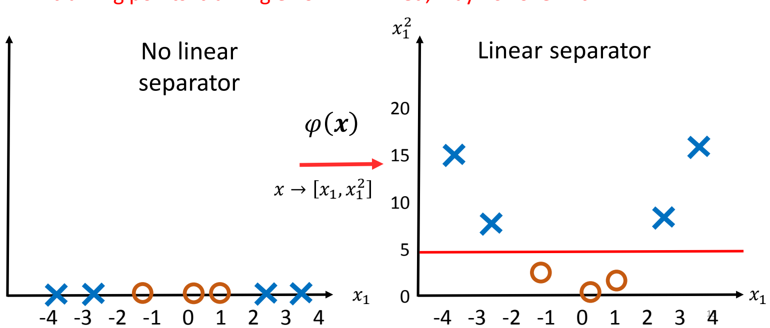
Classifying with additional dimensions

Note: More dimensions makes it easier to separate T training points: training error minimized, may risk over-fit



Quadratic mapping function (math)

$w^T x^k + b = \sum_i \alpha^i y^i (x^i)^T x^k + b$

x_1, x_2, x_3, x_4 -> $x_1, x_2, x_3, x_4, x_1^2, x_2^2, \ldots, x_1x_2, x_1x_3, \ldots, x_2x_4, x_3x_4$

N features -> $N + N + \frac{N\times(N-1)}{2} \approx N^2$ features

N^2 values to learn for w in higher-dimensional space

Or, observe: $(v^T x + 1)^2 = v_1^2 x_1^2 + \cdots + v_N^2 x_N^2$
$+ v_1 v_2 x_1 x_2 + \cdots + v_{N-1} v_N x_{N-1} x_N$
$+ v_1 x_1 + \cdots + v_N x_N$

v with N elements operating in quadratic space

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Quadratic mapping function *Simplified*

x= [x_1, x_2] -> [$\sqrt{2}x_1$, $\sqrt{2}x_2$, x_1^2, x_2^2, $\sqrt{2}x_1x_2$, 1]

x^i=[5,-2] -> [10, -4, 25, 4, -20, 1]   **x**^{k}=[3,-1] -> [6, -2, 9, 1, -6, 1]

$$\varphi(\boldsymbol{x}^i)^T\varphi(\boldsymbol{x}^k) = 30 + 4 + 225 + 4 + 60 + 1 = 324$$

Or, observe: $\left(\boldsymbol{x^i}^T\boldsymbol{x^k} + 1\right)^2 = \left((15+2)+1\right)^2 = (18)^2$ =324

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Mapping function(s)

- Map from low-dimensional space $\boldsymbol{x} = (x_1, x_2)$ to higher dimensional space $\varphi(\boldsymbol{x}) = (\sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2, 1)$
- N data points guaranteed to be separable in space of N-1 dimensions or more

$$\boldsymbol{w} = \sum_i \alpha_i \varphi(\boldsymbol{x^i}) y^i$$

Classifying $\boldsymbol{x^k}$:

$$\sum_i \alpha_i y^i \varphi(\boldsymbol{x^i})^T \varphi(\boldsymbol{x^k}) + b$$

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Kernels

Classifying $\boldsymbol{x^k}$:

$$\sum_i \alpha_i y^i \varphi(\boldsymbol{x^i})^T \varphi(\boldsymbol{x^k}) + b$$

Kernel trick:

- Estimate high-dimensional dot product with function
- $K(\boldsymbol{x^i}, \boldsymbol{x^k}) = \varphi(\boldsymbol{x^i})^T \varphi(\boldsymbol{x^k})$

Now classifying $\boldsymbol{x}^k$

$$\sum_i \alpha_i y^i K(\boldsymbol{x^i}, \boldsymbol{x^k}) + b$$

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Radial Basis Kernel

Try projection to infinite dimensions

$$\varphi(\boldsymbol{x}) = [x_1, \cdots, x_n, x_1^2, \cdots, x_n^2, \cdots, x_1^\infty \cdots, x_n^\infty]$$

Taylor expansion: $e^x = \frac{x^0}{0!} + \frac{x^1}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots + \frac{x^\infty}{\infty!}$

$$K(\boldsymbol{x^i}, \boldsymbol{x^k}) = \exp\left(-\frac{(\boldsymbol{x^i}-\boldsymbol{x^k})^2}{2\sigma^2}\right)$$

Note: $(\boldsymbol{x^i} - \boldsymbol{x^k})^2 = (\boldsymbol{x^i} - \boldsymbol{x^k})^T(\boldsymbol{x^i} - \boldsymbol{x^k})$

Draw separating plane to curve around all support vectors

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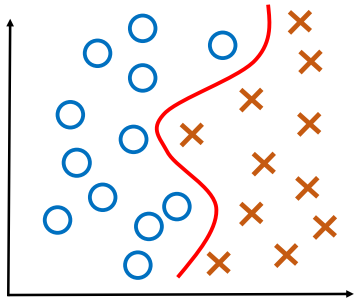
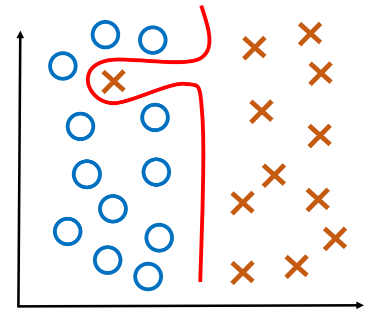
Example RBF-kernel separator



Large margin

Non-linear separation

Potential dangers of RBF-kernel separator



Small margin - **overfitting**

Non-linear separation

The power of SVM (+kernels)

Boundary defined by a few support vectors

- Caused by: maximizing margin
- Causes: less overfitting
- Similar to: regularization

Kernels keep number of learned parameters in check

Binary -> *M*-class classification

- Learn boundary for class *m* vs all other classes
  - Only need M-1 separators for M classes – M^{th} class is for data outside of classes 1, 2, 3, …, M-1
- Find boundary that gives highest margin for data points $\mathbf{x}^i$

Benefits of generative methods

- $P(\boldsymbol{D}|\boldsymbol{\theta})$ and $P(\boldsymbol{\theta}|\boldsymbol{D})$ can generate non-linear boundary

- E.g.: Gaussians with multiple variances